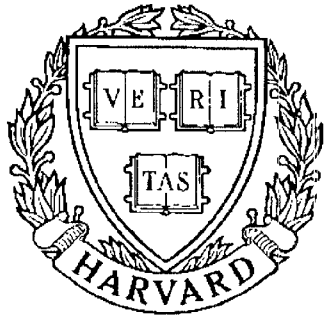
TECHNICAL RESEARCH REPORT

SYSTEMS RESEARCH CENTER



Supported by the National Science Foundation Engineering Research Center Program (NSFD CD 8803012), Industry and the University

Optimal Control of Semi-Batch Processes in the Presence of Modeling Error

by E. Zafiriou and J.M. Zhu

TR 90-21

1990 Amer. Control Conf.
San Diego, CA

Optimal Control of Semi-Batch Processes in the Presence of Modeling Error*

Evanghelos Zafiriou† and Jian-Min Zhu

Chemical Engineering Program
and Systems Research Center
University of Maryland
College Park, MD 20742

Abstract

Batch processes are usually complex and highly nonlinear systems. Modeling error can be the cause of bad performance when optimal input profiles computed for a particular model are applied to the actual plant. The approach followed in this paper uses the available model and actual plant measurements to modify the operation of the next batch, without requiring the remodeling the process. The effect of model error on the convergence of the iterative batch to batch input profile determination is investigated. The method is applied through computer simulations to the determination of the optimal feedrate profile for a cell mass production process. A model parameter update scheme is also proposed, based on the convergence analysis. This is applied to the determination of the optimal temperature profile of bulk polymerization of the optimal temperature profile of styrene.

1 Introduction

Batch processing is becoming increasingly important in the polymerization and biochemical industries. The modeling of such processes often involves complex reaction mechanisms combined with empirical relations. Model plant mismatch always exists, and it may be the cause of bad performance when optimal input profiles computed for a particular model of a semi-batch process are applied to the plant.

To account for such difficulties, we examine an algorithm that directly modifies the input profile $u(t)$ during the course of successive batches. The procedure aims at using information from previous batches to improve the operation of the next without requiring the usually very complex task of remodeling the process. An approximate gradient of an appropriate objective function, *based on both the available model and the measurements obtained from the actual plant*, is computed and then used to find the next input profile, until no further improvement in the objective function can be obtained. In this paper, the proposed approach is demonstrated through computer simulations on a cell mass production process in the presence of modeling error. The effect of model uncertainty on the convergence (from batch to batch) is also considered. A convergence analysis after each iteration may be used to help modify the values of certain model parameters, if so desired. This procedure is demonstrated on the problem of determining the minimum-time temperature profile for the batch bulk polymerization of styrene. The methodology can be applied on any systems operated in semi-batch mode, regardless of their nature.

*Supported in part by the National Science Foundations's Engineering Research Centers Program : NSFD CDR 8803012.

†Author to whom correspondence should be addressed. E-mail: zafiriou@cacse.src.umd.edu

2 Iterative Batch-to-Batch Input Profile Determination

2.1 Methodology

The approach was introduced in [7] and it is based on the analogy between the iterations during the numerical optimization of the appropriate cost functional (objective function) on one hand and the successive batches during the operation of the plant on the other. A gradient computation after every batch is required. The gradient computation in numerical optimization involves two integrations. The first forward integration of the nonlinear differential equations that describe the plant, is not carried out numerically in this approach, but rather it is carried by the actual plant itself, its result being the plant measurements. Note that since these measurements are not used for on-line control, no instantaneous measurements are required. For example, samples of the product can be collected during the course of the batch and sent for analysis. The second backward integration of the adjoint system, however, requires the use of the process model. The result of the above procedure will be an estimate for the gradient, defined as $\tilde{g}(t)$. This $\tilde{g}(t)$ is then used to compute the search direction that will result in the next input profile, so that a steady improvement in performance is accomplished from batch to batch. This technique is shown in Table 1. Step 5 uses the steepest

Table 1: Analogy between Numerical Optimization and Plant Operation

NUMERICAL OPTIMIZATION	PLANT OPERATION
$\min_{u(t)} \phi(x(t_f))$ where $\dot{x} = f(x,u)$, $x(0) = x_0$ (model)	$\min_{u(t)} \phi(x(t_f))$ where $\dot{x} = \tilde{f}(x,u)$, $x(0) = x_0$ (plant)
1st iteration	1st batch
1. Forward integration of model $u_1(t) \rightarrow \dot{x} = f(x,u)$, (model) $\rightarrow x_1(t)$	1. Forward integration of plant $u_1(t) \rightarrow \dot{x} = \tilde{f}(x,u)$, (plant) $\rightarrow \check{x}_1(t)$ (off-line measurement)
2. Linearize model $f(x,u)$ at u_1, x_1 $u_1(t), x_1(t) \rightarrow$ Linearization $\rightarrow f_x(x_1,u_1)$ $u_1(t), x_1(t) \rightarrow$ Linearization $\rightarrow f_u(x_1,u_1)$	2. Linearize model $f(x,u)$ at $u_1, \check{x}_1$ $u_1(t), \check{x}_1(t) \rightarrow$ Linearization $\rightarrow f_x(\check{x}_1,u_1)$ $u_1(t), \check{x}_1(t) \rightarrow$ Linearization $\rightarrow f_u(\check{x}_1,u_1)$
3. Backward integration of adjoint system $\dot{\lambda} = -f_x(x_1,u_1)\lambda$; $\lambda(t_f) = \nabla_x \phi(x_1(t_f))$	3. Backward integration of approximate adjoint system $\dot{\check{\lambda}} = -f_x(\check{x}_1,u_1)\check{\lambda}$; $\check{\lambda}(t_f) = \nabla_x \phi(\check{x}_1(t_f))$
4. Gradient $g(t) = f_u^T(x_1,u_1)\lambda(t)$	4. Estimate gradient $\check{g}(t) = f_u^T(\check{x}_1,u_1)\check{\lambda}(t)$
5. Line search Search direction : $s(t) = -Pg(t)$ P : constraint projection matrix $u_2(t) = u_1(t) + \alpha s(t)$ $0 \leq \alpha \leq \alpha_{max}$ where α_{max} is the limit imposed by constraints. For every α, step 1 has to be repeated, until the line search is terminated.	5. Line search Search direction: $\check{s}(t) = -P\check{g}(t)$ P : constraint projection matrix $u_2(t) = u_1(t) + \alpha\check{s}(t)$ $0 \leq \alpha \leq min[\alpha_e, \alpha_{max}]$ where α_{max} is the limit imposed by constraints; and α_e is a limit on maximum adjustment of actual plant. For every α, step 1 has to be repeated, until the line search is terminated.

descent with constraints method. This method is known to be rather slow close to the optimum. However, if one starts far from the optimum, it produces fast improvement. This is exactly what one needs right after a change has moved the process far from optimal operation. Other techniques can of course be used as well. The line search over α terminates as soon as an improvement is obtained. Note that to obtain the value of the objective function for a particular α, the corresponding input profile has to be implemented to the actual plant. It should be noted that because of this line search, one may occasionally have a temporary increase in the performance index, although $\check{s}(t)$ may be a valid descent direction for the actual plant.

2.2 A Fed-Batch Fermentation Example

We consider the cell mass production problem described in [4,6]. The original problem is singular, but a change of the optimization variable from flowrate to volume and discretization of (5) below results in a non-singular problem [5]:

$$min \;\; J = -XV(t_f) \tag{1}$$

$$\frac{d}{dt}(XV) = \mu XV \tag{2}$$

$$\frac{d}{dt}((S_F - S)V) = \sigma XV \tag{3}$$

$$V_{min} \leq V \leq V_{max} \tag{4}$$

$$0 \leq \frac{dV}{dt} \leq F_{max} \tag{5}$$

$$\mu(S) = [0.504S(1 - 0.0204S)]/[0.00849 + S + 0.0406S^2] \tag{6}$$

$$Y(S) = [0.383(1 - 0.0204S)]/[1 + 0.296S - 0.00501S^2] \tag{7}$$

$$\sigma(S) = \mu(S)/Y(S) \tag{8}$$

where X and S are cell mass and substrate concentration; F and V are flowrate and volume respectively.

The optimal volume profile $V(t)$ is shown in Fig. 3 (dotted line), where $(XV)_0 = 1g, (SV)_0 = 5g, (V)_0 = 1L, V_{max} = 5L, F_{max} = 4L/h, S_F = 10g/L, t_f = 6h, J(V^*) = -16.304$, the subscripts 0 and F denoting initial conditions and feed stream respectively. The above case is defined as nominal for the following simulations.

We emulate model-plant mismatch by introducing error in (7) , which describes the relationship between the yield coefficient and the substrate concentration. Figure 1 shows the experimental data given in the literature [1] and a plot of (7). To emulate the model error, we will assume that $Y(S)$ for the true plant is given by the dotted line in Fig 1. This corresponds to introducing an uncertain parameter k in the yield expression:

$$Y(S) = [0.383(1 - 0.0204S)]/[1 + 0.296kS - 0.00501S^2] \tag{9}$$

Fig. 1 shows yield curves of (9) with k=1 (model), k=3 (plant).

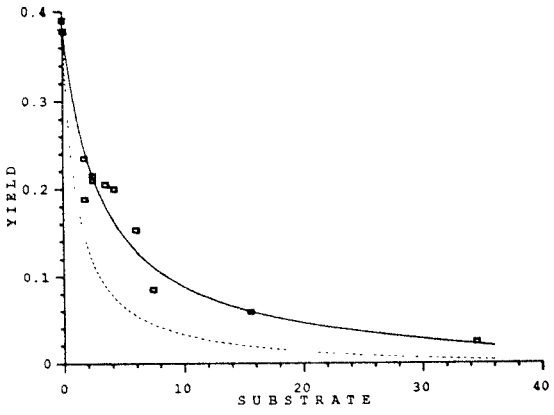


Figure 1: Yield; solid line: k=1; dotted line: k=3 ; squares: experimental points.

The steepest descent with constraints method is used, as described in Table 1. An additional limit on the maximum adjustment from batch to batch for the control variable is introduced to avoid radical changes that may be unacceptable in an industrial environment. In this case, we impose a limit of $0.1F_{max}$ on the change of the flowrate F , which corresponds to α_e.

Figure 2 demonstrates that the proposed algorithm can provide a significant improvement in the performance index (computed for the actual plant) even if a mismatch between the model (k=1) and the plant (k=3) exists. For comparision, the initial volume profile ($J = -13.715$) computed from the model, the volume profile $V(t)$ obtained through our procedure ($J = -15.678$) and the true optimal profile for the plant (if the true plant equations were known; $J = -15.689$) are shown in Fig. 3.

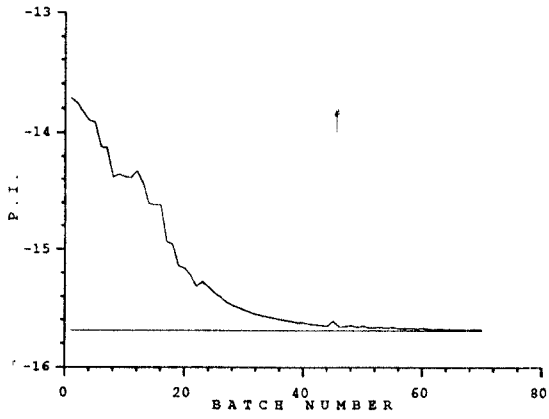


Figure 2: Plant operation under model-plant mismatch

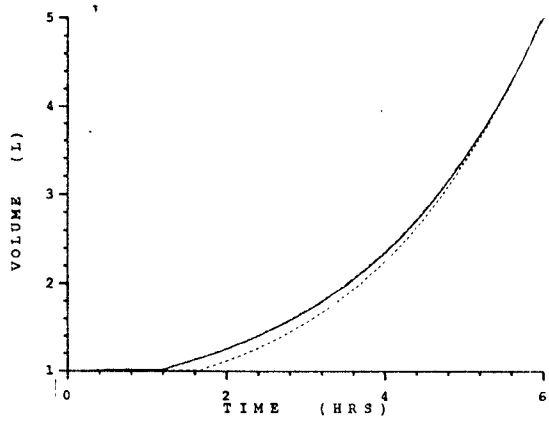


Figure 3: Volume Profiles; solid line: volume profile after 70 batches; dotted line: initial volume profile; dash-dot line (coincides with solid): true optimal volume profile

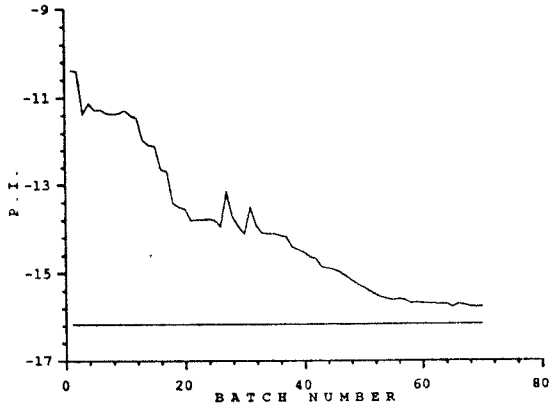


Figure 4: Plant operation under initial conditions error

The effect of error in the assumed initial conditions is similar to that of model error, since only an approximation of the gradient of the true plant is available. The plant operation under initial conditions error (assumed: $X_0 = 1, S_0 = 5$; true: $X_0 = 1, S_0 = 1$) with initial $V(t)$ the optimal for the nominal case is shown in Fig. 4.

Finally, Fig. 5 describes the plant operation in the presence of both model-plant mismatch, (model k=1, plant k=3), initial condition error (assumed: $X_0 = 1, S_0 = 5$; true: $X_0 = 1, S_0 = 1$) and 10% measurement error (or estimation error) in the state variables X and S.

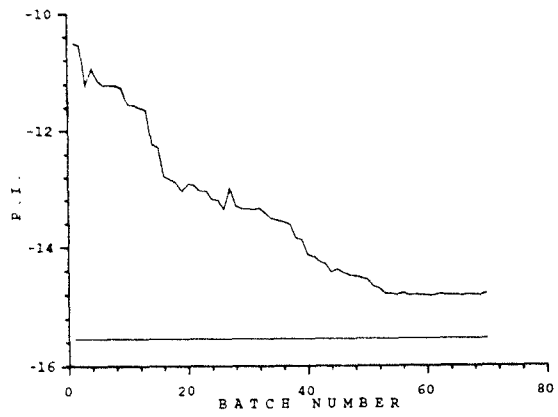


Figure 5: Plant operation under model-plant mismatch, initial condition error and 10% measurement error in the state variables X and S.

3 Convergence Analysis and Model Modification

3.1 Robust Convergence Condition

This section attempts to quantify the effect of model uncertainty on the convergence (from batch to batch) of the proposed procedure. Since the computation of the search direction is based on an approximate gradient, if the model error is too large, it may not be a descent direction. In order to have a descent property, we need:

$$< -g_{plant}(t), \tilde{s}(t) > \quad > 0 \qquad (10)$$

where $g_{plant}(t)$ is the gradient for the true plant equations and

$$< f_1(t), f_2(t) > \stackrel{\text{def}}{=} \int_0^{t_f} f_1(t) f_2(t) \quad dt \qquad (11)$$

Since $g_{plant}(t)$ is unknown, a robustness condition for convergence can be obtained by requiring that the above condition be satisfied for the infimum over all possible plant parameter values.

Consider the optimal control problem defined in the left column of Table 1. Let K be a vector of uncertain parameters, for which lower and upper limits are known. Different values of K result in different f_x and f_u, i.e., $f_x = f_x(x, u; K)$ and $f_u = f_u(x, u; K)$. (f_x, f_u are the partial derivatives of f w.r.t. x, u.) When the procedure of the left column of Table 1 is used for different K, we will obtain different gradients that depend on K: $g(t) = g(t; K)$. The gradient for the true plant is the one that corresponds to the true value of K:

$$g_{plant}(t) = g(t; K_{true}) \qquad (12)$$

When, during the iterative batch-to-batch determination of the input profile, a new search direction has been determined (according to the right column of Table 1), then (10) and (12) can be combined to yield:

$$\inf_K < -g(t; K), \tilde{s}(t) > \quad > 0 \qquad (13)$$

Satisfaction of (13) guarantees that $\tilde{s}(t)$ is a descent direction for any possible plant. This condition however may be difficult to satisfy because of its inherent conservativeness. This is due to the fact that $\tilde{s}(t)$ corresponds to the "true" value of K, whose effect on $\tilde{s}(t)$ comes from step 1 of the procedure (right column of Table 1). Hence it may very well be a descent direction for that particular K_{true}, if $< -g(t; K_{true}), \tilde{s}(t) >$ is positive, while (13) is not satisfied.

We suggest that $\tilde{s}(t)$ be implemented even if (13) is not satisfied. If the line search results in an improvement, this means that (10) is satisfied for the true plant. This information can be used to improve the model by modifying the value for K and narrowing down the region of possible values. For one parameter this would work as follows. Let the possible values of K lie in $[K_{low}, K_{high}]$, and (13) not be satisfied for all of them, but only for the smaller set $\Omega = [\omega_1, \omega_2] \subset [K_{low}, K_{high}]$. Since $\tilde{s}(t)$ has proved from the actual plant data to be a descent direction, K_{true} must lie in Ω. This interval can now become the new (and smaller) $[K_{low}, K_{high}]$. If the value of K used in the model is not in Ω, then it is modified and set to either ω_1 or ω_2, whichever is closest to the previous value. This technique is illustrated with an example in the following section. For more than one uncertain parameters, the method is conceptually the same, but the construction of the set Ω is a more challenging task.

3.2 A Bulk Polymerization Example

The thermally initiated bulk polymerization of styrene was modeled by Kwon and Evans [2] through reaction mechanism analysis and laboratory tests. The control objective is to find the optimal temperature profile that minimizes the batch time required to reach the specified conversion (80%) and polymer properties (final specific number average chain length ($NACL$) and weight average chain length ($WACL$) equal to 1). A coordinate transformation changes the problem into a fixed end-time optimization with the conversion acting as the new "time" coordinate [3]. The methodology described in Table 1 can then be applied.

We emulate model-plant mismatch by introducing error in the parameters of the empirical relation between the properties of newly formed increment of polymer and temperature:

$$\bar{x}_w^0 = A_w exp(B/T) \qquad (14)$$

where $\bar{x}_w^0$ is the $WACL$ formed at the current absolute temperature T. This is an empirical relationship and the coefficients A_w and B are obtained experimentally [2,3]. The procedure of section 2.1 was applied to this system for a number of different modeling errors in [8]. The case for 50% error in A_w is shown in Fig. 6 (dotted line). Clearly this was sufficient to cause a very large error in the optimal value of the reaction time. The methodology led to the true optimum in about 5 batches without modifying the inaccurate model. More details can be found in [8]. Note that the maximum adjustment $(\Delta T)_{max}$ (which determines α_ϵ in Table 1) is selected 5^0C, and varies with the difference ΔJ in the performance index J between the end results of the last two line searches (which are carried out as described in the right column of Table 1):

$$(\Delta T)_{max} = \begin{cases} 5^0C & \text{if } |\Delta J| \geq 50 \\ 2^0C & \text{if } 1 \leq |\Delta J| < 50 \\ 1^0C & \text{if } |\Delta J| < 1 \end{cases}$$

In this section we examine the outcome of applying the analysis of section 3.1 on this example. The results are shown in Table 2 and Fig. 6. We consider two cases. In both the error lies in A_w. In the first case the robust convergence condition is correctly computed over possible values of A_w and its value in the model is appropriately modified, when needed. In the second case, we assume that the uncertain parameter is B, and proceed with modifying its value, although the error is in A_w.

Let us consider the two cases carefully. In the first, $K = K_a$ and the initial $[K_{low}, K_{high}] = [0.050, 2.500]$ with $K_{true} = 1.5$. Everytime a line search over a new search direction $\bar{s}(t)$ is completed, the set Ω is constructed and the value of K_a in the model is appropriately modified, if not already in Ω. Note that the numbers in the first column of Table 2 correspond to the number of line searches made and not to the number of batches, since each line search, as mentioned in Table 1, usually requires more than one batch. The coordinate in Fig. 6 though, corresponds to number of batches. As it can be seen from Table 2, K_a eventually converges towards the true value 1.50. At the same time, Fig. 6 shows a small improvement in the speed of convergence towards the true optimal operating policy.

In the second case we have $K = K_b$ and start with $[K_{low}, K_{high}] = [0.900, 1.200]$. In this case, however, there is no way to define K_{true}, since we incorrectly assume the error is in B, instead of A_w. This is a situation that one would expect to occur in practice often. This case is used as a test of "robustness" of the method to this kind of incorrect assumptions. Table 2 shows that the value of K_b in the model is modified. At the same time, Fig. 6 shows that this creates no problems, and that it actually speeds up the convergence to the true optimal opearting policy as much as in the first case.

Table 2: Plant: $A'_w = 1.50 A_w \quad B' = B$

	Modify A_w		Modify B	
	$A'_w = K_a A_w \quad B' = B$		$A'_w = A_w \quad B' = K_b B$	
	$K_a \in [0.050, 2.500]$		$K_b \in [0.900, 1.200]$	
No.	Ω_a^i	K_a^i	Ω_b^i	K_b^i
1		1.000		1.000
2	[1.109, 2.500]	1.109	[1.010, 1.200]	1.010
3	[1.229, 2.500]	1.229	[1.019, 1.200]	1.019
4	[1.368, 2.500]	1.368	[1.028, 1.200]	1.028
5	[1.368, 1.516]	1.368	[1.028, 1.038]	1.028
6	[1.368, 1.516]	1.368	[1.028, 1.038]	1.028
7	[1.483, 1.516]	1.483	[1.028, 1.038]	1.028
8	[1.483, 1.511]	1.483	[1.028, 1.038]	1.028
9	[1.483, 1.511]	1.483	[1.028, 1.038]	1.028
10	[1.492, 1.511]	1.492	[1.028, 1.038]	1.028

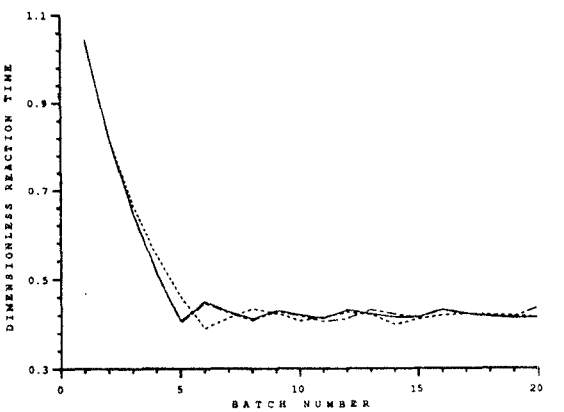


Figure 6: 50% error in A_w. Dotted line: no model modification; dash-dot: modify A_w; solid: modify B.

4 Conclusion

A method that directly modifies the input trajectory for a semi-batch process from batch to batch, in order to correct for model error, has been successfully tested through computer simulations on a biochemical cell mass production system. It was shown that although the model is never changed, eventually we obtain the input profile that is optimal for the true plant. This is accomplished by combining the available model with plant measurements to get an estimate of the objective function gradient which, although not accurate, is still a descent direction, thus producing an improvement in every batch. The methodology behaves equally well in the case of error in the initial conditions assumptions and in the presence of

measurement errors.

A condition was also developed that guarantees that the gradient estimate is indeed a descent direction for every possible value of the uncertain parameters of the system. This condition is sufficient only, and thus conservative. When it is not satisfied, this fact can be used to narrow down the region of uncertainty and modify the parameter values in the model. This technique was successfully applied to simulations of a thermally initiated bulk polymerization of styrene. Further work is needed in order to provide a computationally efficient procedure for the multi-parameter case.

References

[1] D. Dibiasio, H. C. Lim and W. A. Weigand, "An Experimental Investigation of Stability and Multiplicity of Steady States in a Biological Reactor," AIChE Journal, **27**, pp. 284–292, 1981.

[2] Y. D. Kwon and L. B. Evans," Continuous Blending Models for Free Radical Polymerization Systems," Can. J. Chem. Eng., **51**,p. 71, 1973.

[3] Y. D. Kwon and L. B. Evans, "A Coordinate Transformation Method for the Numerical Solution of Non-linear Minimum-time Control Problems," AIChE. J., **21**, p. 1158, 1975.

[4] J. M. Modak and H. C. Lim, "Feedback Optimization of Fed-Batch Fermentation," Biotechnol. Bioeng., **30**, pp. 528–540, 1987.

[5] J. M. Modak and H. C. Lim, "Simple Nonsingular Control Approach to Fed-Batch Fermentation Optimization," Biotechnol. Bioeng., **33**, pp. 11–15, 1989.

[6] S. J. Parulekar, J. M. Modak and H. C. Lim, "Optimal Control of Fed-Batch Bioreactors," Proc. of the Amer. Control Conf., p. 849, Boston, MA, 1985.

[7] E. Zafiriou and J.-M. Zhu,"Optimal Feed-Rate Profile Determination for Fed-batch Fermentations in the Presence of Model-Plant Mismatch," Proc. of the Amer. Control Conf., p. 2006-2009, Pittsburgh, PA, June 1989.

[8] J.-M. Zhu and E. Zafiriou, "Iterative Batch-to-Batch Input Profile Determination for Semi-Batch Processes–A Polymerization Example," AIChE Ann. Meeting, Paper for Poster No. 167Bp, San Francisco, CA, Nov. 1989